



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 AM GMT

PDB ID : 3HYR
Title : Structural Insight into G Protein Coupling and Regulation of Fe²⁺ Membrane Transport
Authors : Maher, M.J.; Jormakka, M.
Deposited on : 2009-06-23
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

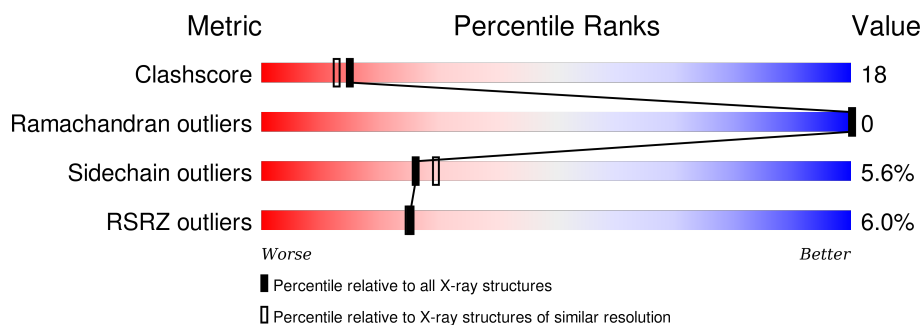
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	<div> <div>4%</div> <div>66% 25% 6%</div> </div>
1	B	270	<div> <div>4%</div> <div>69% 23% 6%</div> </div>
1	C	270	<div> <div>8%</div> <div>68% 23% 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferrous iron transport protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	Se	0	5	0
			1953	1229	340	374	6	4			
1	B	253	Total	C	N	O	S	Se	0	4	0
			1944	1221	340	373	6	4			
1	C	253	Total	C	N	O	S	Se	0	4	0
			1944	1221	340	373	6	4			

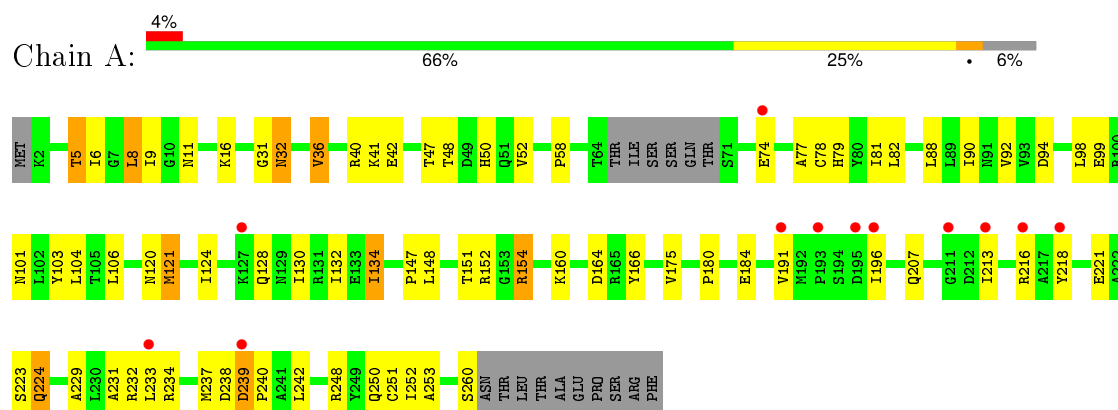
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total	O	0	0
			152	152		
2	B	173	Total	O	0	0
			173	173		
2	C	155	Total	O	0	0
			155	155		

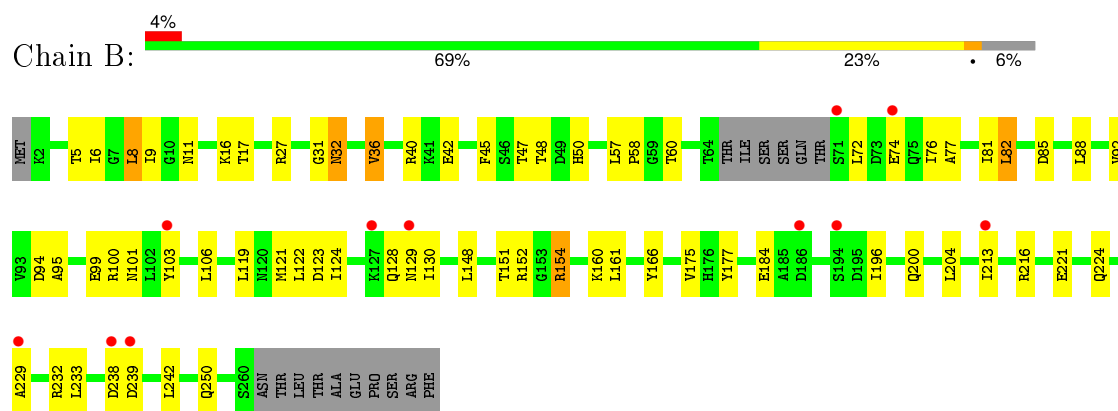
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

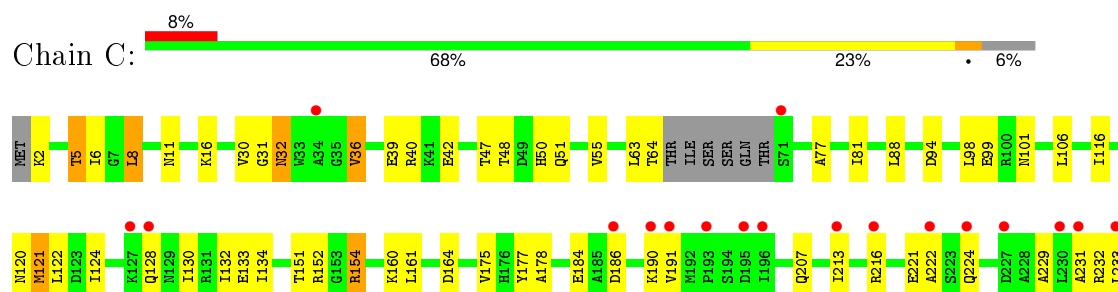
• Molecule 1: Ferrous iron transport protein B

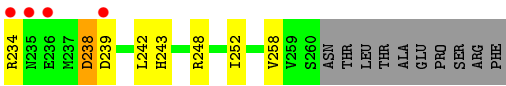


• Molecule 1: Ferrous iron transport protein B



• Molecule 1: Ferrous iron transport protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.12Å 84.44Å 66.24Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 69.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.20) 99.9 (69.30-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.225 , 0.287 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 38843 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6321	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/1990	0.72	2/2698 (0.1%)
1	B	0.63	0/1977	0.74	3/2680 (0.1%)
1	C	0.60	0/1977	0.72	1/2680 (0.0%)
All	All	0.61	0/5944	0.73	6/8058 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	154	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	154	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	154	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	154	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	148	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1953	0	1985	75	0
1	B	1944	0	1976	73	0
1	C	1944	0	1976	68	0
2	A	152	0	0	30	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	173	0	0	36	0
2	C	155	0	0	29	0
All	All	6321	0	5937	207	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:HB3	2:C:408:HOH:O	1.53	1.08
1:A:191:VAL:HB	2:A:332:HOH:O	1.53	1.05
1:C:191:VAL:HB	2:C:361:HOH:O	1.57	1.02
1:B:45:PHE:HB3	2:B:425:HOH:O	1.59	1.02
1:A:31:GLY:HA3	2:A:334:HOH:O	1.64	0.97
1:B:72:LEU:HD22	2:B:336:HOH:O	1.63	0.97
1:B:196:ILE:HG21	2:B:455:HOH:O	1.66	0.94
2:A:388:HOH:O	1:B:161:LEU:HD22	1.67	0.92
1:A:251:CYS:HA	2:A:388:HOH:O	1.70	0.91
1:B:45:PHE:CD2	2:B:425:HOH:O	2.22	0.91
1:A:148:LEU:HD12	2:A:351:HOH:O	1.68	0.90
1:A:32:ASN:HB3	2:A:370:HOH:O	1.71	0.88
1:C:77:ALA:O	1:C:81:ILE:HG12	1.74	0.87
1:A:77:ALA:O	1:A:81:ILE:HG12	1.74	0.87
1:B:47[B]:THR:HG23	1:B:160:LYS:HB3	1.56	0.86
1:B:77:ALA:O	1:B:81:ILE:HG12	1.77	0.85
1:A:52:VAL:HG13	2:A:284:HOH:O	1.77	0.84
1:C:47[B]:THR:HG23	1:C:160:LYS:HB3	1.58	0.82
1:A:250:GLN:HA	2:A:308:HOH:O	1.78	0.82
1:C:234:ARG:HB2	2:C:310:HOH:O	1.79	0.81
1:B:106:LEU:HB2	2:B:290:HOH:O	1.81	0.80
1:B:31:GLY:HA3	2:B:337:HOH:O	1.81	0.80
1:C:30:VAL:HG13	2:C:458:HOH:O	1.81	0.80
1:C:39:GLU:HG3	2:C:458:HOH:O	1.82	0.80
1:A:154:ARG:HH22	1:C:99:GLU:CD	1.85	0.80
1:A:154:ARG:NH2	1:C:99:GLU:OE2	2.17	0.78
1:B:9:ILE:HD12	2:B:410:HOH:O	1.83	0.77
1:C:231:ALA:HA	2:C:310:HOH:O	1.85	0.77
1:C:232:ARG:HG2	2:C:278:HOH:O	1.85	0.76
1:B:99:GLU:CD	1:C:154:ARG:HH22	1.89	0.75
1:B:123:ASP:HB2	2:B:340:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47[A]:THR:CG2	1:C:50:HIS:HB2	2.18	0.74
1:A:234:ARG:HG3	2:A:393:HOH:O	1.87	0.74
1:A:47[B]:THR:HG23	1:A:160:LYS:HB3	1.70	0.73
1:B:47[A]:THR:CG2	1:B:50:HIS:HB2	2.19	0.73
1:B:88:LEU:HD22	2:B:389:HOH:O	1.89	0.73
1:A:196:ILE:HD11	1:A:218[B]:TYR:CD2	2.24	0.73
1:A:99:GLU:CD	1:B:154:ARG:HH22	1.93	0.72
1:A:253:ALA:HB3	2:A:308:HOH:O	1.91	0.71
1:A:47[A]:THR:CG2	1:A:50:HIS:HB2	2.21	0.71
1:C:133:GLU:HG3	2:C:357:HOH:O	1.91	0.71
1:B:6:ILE:HG12	1:B:88:LEU:HD23	1.74	0.70
1:B:32:ASN:HB2	2:B:363:HOH:O	1.90	0.69
1:B:88:LEU:CB	2:B:389:HOH:O	2.40	0.69
1:C:243:HIS:CE1	2:C:370:HOH:O	2.45	0.68
1:B:45:PHE:HD2	2:B:425:HOH:O	1.66	0.68
1:C:47[A]:THR:HG22	1:C:50:HIS:HB2	1.76	0.68
1:B:124:ILE:HD12	2:B:340:HOH:O	1.93	0.68
1:B:58:PRO:HB2	2:B:315:HOH:O	1.93	0.67
1:A:32:ASN:OD1	1:A:36:VAL:O	2.13	0.66
1:B:88:LEU:HB2	2:B:389:HOH:O	1.96	0.65
1:B:85:ASP:OD2	2:B:468:HOH:O	2.13	0.65
1:A:196:ILE:HD11	1:A:218[B]:TYR:HD2	1.60	0.65
1:A:58:PRO:HB2	2:A:299:HOH:O	1.98	0.64
1:B:129:ASN:ND2	2:B:285:HOH:O	2.30	0.64
1:C:32:ASN:OD1	1:C:36:VAL:O	2.16	0.64
2:A:388:HOH:O	1:B:161:LEU:CD2	2.35	0.63
1:C:151:THR:HG22	1:C:152:ARG:HG3	1.81	0.63
1:B:47[A]:THR:HG22	1:B:50:HIS:HB2	1.81	0.63
1:A:99:GLU:OE2	1:B:154:ARG:NH2	2.32	0.63
1:C:8:LEU:HD13	1:C:16:LYS:HG3	1.81	0.62
1:B:8:LEU:HD13	1:B:16:LYS:HG3	1.81	0.62
1:A:196:ILE:CD1	1:A:218[B]:TYR:HD2	2.13	0.61
1:B:99:GLU:OE2	1:C:154:ARG:NH2	2.34	0.61
1:A:47[A]:THR:HG22	1:A:50:HIS:HB2	1.81	0.61
1:A:47[A]:THR:HG23	1:A:50:HIS:H	1.66	0.60
1:B:32:ASN:OD1	1:B:36:VAL:O	2.19	0.60
1:A:147:PRO:HG3	2:C:451:HOH:O	2.01	0.60
1:C:213:ILE:HG23	1:C:216:ARG:HH11	1.67	0.60
1:C:47[B]:THR:HG22	2:C:285:HOH:O	2.01	0.60
1:B:17:THR:HA	2:B:318:HOH:O	2.00	0.60
1:A:120:ASN:CG	2:A:351:HOH:O	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47[A]:THR:HG23	1:C:50:HIS:H	1.67	0.60
1:B:57:LEU:HD13	2:B:410:HOH:O	2.01	0.60
1:B:103:TYR:HD1	2:B:423:HOH:O	1.83	0.60
1:A:184:GLU:OE1	1:A:232:ARG:NH1	2.35	0.59
1:A:41:LYS:HE2	2:A:374:HOH:O	2.03	0.58
1:A:148:LEU:CD1	2:A:351:HOH:O	2.38	0.57
1:C:222:ALA:HA	2:C:361:HOH:O	2.04	0.57
1:A:213:ILE:HG23	1:A:216:ARG:HH11	1.70	0.57
1:A:78:CYS:HB3	2:A:419:HOH:O	2.05	0.57
1:B:213:ILE:HG23	1:B:216:ARG:HH11	1.70	0.57
1:B:128:GLN:HE21	1:B:130:ILE:CD1	2.19	0.56
1:C:234:ARG:HG3	2:C:352:HOH:O	2.05	0.56
1:B:196:ILE:CG2	2:B:455:HOH:O	2.35	0.55
1:B:47[B]:THR:HG22	2:B:294:HOH:O	2.07	0.55
1:C:258:VAL:HA	2:C:451:HOH:O	2.05	0.55
1:A:47[B]:THR:HG22	2:A:337:HOH:O	2.06	0.55
1:A:94:ASP:OD2	1:A:121:MSE:HG3	2.07	0.54
1:B:47[A]:THR:HG23	1:B:50:HIS:H	1.72	0.54
1:B:184:GLU:OE1	1:B:232:ARG:NH1	2.40	0.54
1:C:184:GLU:OE1	1:C:232:ARG:NH1	2.41	0.54
1:A:11:ASN:HD21	1:A:101:ASN:HA	1.72	0.54
1:C:31:GLY:HA3	2:C:271:HOH:O	2.08	0.54
1:A:47[B]:THR:HG22	1:A:48:THR:H	1.73	0.54
1:A:6:ILE:HG12	1:A:88:LEU:HD23	1.89	0.54
1:A:248:ARG:HD3	2:A:387:HOH:O	2.07	0.54
1:B:77:ALA:HB1	2:B:410:HOH:O	2.07	0.54
1:C:55:VAL:HG21	2:C:326:HOH:O	2.08	0.54
1:B:151:THR:CG2	2:B:307:HOH:O	2.55	0.53
1:A:106:LEU:HD13	2:A:339:HOH:O	2.06	0.53
1:B:72:LEU:CD2	2:B:336:HOH:O	2.38	0.53
1:A:8:LEU:HD13	1:A:16:LYS:HG3	1.90	0.53
1:B:16:LYS:HB2	1:B:92[B]:VAL:HG11	1.90	0.53
1:C:128:GLN:HE21	1:C:130:ILE:CD1	2.22	0.53
1:C:221:GLU:O	1:C:224:GLN:HG2	2.08	0.53
1:A:250:GLN:NE2	1:B:161:LEU:HB2	2.23	0.53
1:B:47[B]:THR:HG22	1:B:48:THR:H	1.74	0.53
1:B:151:THR:HG21	2:B:307:HOH:O	2.08	0.53
1:B:11:ASN:ND2	2:B:292:HOH:O	2.34	0.53
1:C:128:GLN:HE21	1:C:130:ILE:HD11	1.74	0.52
1:B:151:THR:HG22	1:B:152:ARG:HG3	1.91	0.52
1:A:50:HIS:HE1	2:A:340:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLN:HE21	1:B:130:ILE:HD11	1.74	0.52
1:C:94:ASP:OD2	1:C:121:MSE:HG3	2.08	0.52
1:B:221:GLU:O	1:B:224:GLN:HG2	2.09	0.52
1:C:47[A]:THR:OG1	1:C:164:ASP:OD2	2.28	0.52
1:B:204:LEU:HD12	2:B:455:HOH:O	2.10	0.52
1:C:184:GLU:HG3	1:C:229:ALA:HB1	1.91	0.52
1:A:184:GLU:HG2	1:A:233:LEU:HG	1.92	0.51
1:B:47[A]:THR:HG21	1:B:50:HIS:HB2	1.92	0.51
1:C:184:GLU:HG2	1:C:233:LEU:HG	1.93	0.51
1:B:11:ASN:HD21	1:B:101:ASN:HA	1.76	0.51
1:B:184:GLU:HG3	1:B:229:ALA:HB1	1.93	0.51
1:C:63:LEU:HA	2:C:320:HOH:O	2.10	0.51
1:A:221:GLU:O	1:A:224:GLN:HG2	2.11	0.50
1:B:94:ASP:OD2	1:B:121:MSE:HG3	2.11	0.50
1:A:128:GLN:HE21	1:A:130:ILE:CD1	2.25	0.50
1:C:2:LYS:HE3	2:C:345:HOH:O	2.11	0.50
1:B:40:ARG:HH12	1:B:42:GLU:CD	2.15	0.50
1:C:178:ALA:HB2	2:C:400:HOH:O	2.11	0.50
1:A:180:PRO:HB2	1:A:237:MSE:CE	2.42	0.50
1:C:47[B]:THR:HG22	1:C:48:THR:H	1.76	0.50
1:A:184:GLU:HG3	1:A:229:ALA:HB1	1.94	0.49
1:A:223:SER:HB3	2:A:442:HOH:O	2.13	0.49
1:A:128:GLN:HE21	1:A:130:ILE:HD11	1.76	0.49
1:C:31:GLY:N	2:C:458:HOH:O	2.44	0.49
1:C:11:ASN:HD21	1:C:101:ASN:HA	1.78	0.49
1:C:186:ASP:HB3	2:C:382:HOH:O	2.12	0.48
1:B:88:LEU:CD2	2:B:389:HOH:O	2.56	0.48
1:A:196:ILE:CD1	1:A:218[B]:TYR:CD2	2.92	0.48
1:B:76:ILE:HG13	2:B:336:HOH:O	2.12	0.48
1:A:151:THR:HG22	1:A:152:ARG:HG3	1.96	0.48
1:B:200:GLN:NE2	2:B:357:HOH:O	2.46	0.47
1:B:82:LEU:CD1	2:B:357:HOH:O	2.61	0.47
1:B:184:GLU:HG2	1:B:233:LEU:HG	1.95	0.47
1:C:234:ARG:NH1	2:C:352:HOH:O	2.47	0.47
1:A:260:SER:CB	2:A:347:HOH:O	2.62	0.47
1:A:47[A]:THR:HG21	1:A:50:HIS:HB2	1.96	0.47
1:A:207:GLN:HE22	1:A:248:ARG:HH21	1.63	0.46
1:A:231:ALA:HB2	2:A:429:HOH:O	2.14	0.46
1:B:152:ARG:NE	2:B:307:HOH:O	2.49	0.46
1:A:79:HIS:HE1	2:A:382:HOH:O	1.98	0.46
1:B:175:VAL:HG11	1:B:177:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:HA	2:A:284:HOH:O	2.16	0.46
1:A:47[A]:THR:HG23	1:A:50:HIS:N	2.31	0.46
1:C:258:VAL:HG22	2:C:451:HOH:O	2.16	0.45
1:B:9:ILE:HA	2:B:364:HOH:O	2.17	0.45
1:A:16:LYS:HB2	1:A:92[B]:VAL:HG11	1.99	0.45
1:A:58:PRO:HD3	2:A:390:HOH:O	2.17	0.45
1:C:207:GLN:HE22	1:C:248:ARG:HH21	1.65	0.45
1:C:5:THR:HG21	2:C:335:HOH:O	2.16	0.44
1:A:132:ILE:O	1:A:134:ILE:HD12	2.18	0.44
1:C:238:ASP:N	2:C:370:HOH:O	2.51	0.44
1:C:6:ILE:HG12	1:C:88:LEU:HD23	2.00	0.44
1:B:106:LEU:HD21	1:B:175:VAL:CG2	2.48	0.43
1:B:95:ALA:HB2	1:B:119:LEU:HD22	1.99	0.43
1:A:47[B]:THR:HG21	1:A:160:LYS:O	2.18	0.43
1:C:98:LEU:HD22	1:C:132:ILE:HD12	2.00	0.43
1:A:196:ILE:HD11	1:A:218[B]:TYR:CE2	2.53	0.43
1:A:120:ASN:C	1:A:121:MSE:HG2	2.39	0.43
1:A:47[A]:THR:HG1	1:A:164:ASP:CG	2.22	0.43
1:A:6:ILE:HG21	1:A:90:ILE:HD12	2.00	0.43
1:C:175:VAL:HG11	1:C:177:TYR:CZ	2.54	0.43
1:C:64:THR:HA	2:C:421:HOH:O	2.17	0.43
1:A:40:ARG:HH12	1:A:42:GLU:CD	2.21	0.43
1:C:47[A]:THR:HG23	1:C:50:HIS:N	2.31	0.42
1:B:99:GLU:OE1	1:C:154:ARG:NH2	2.46	0.42
1:C:47[B]:THR:CG2	1:C:160:LYS:HB3	2.41	0.42
1:A:47[A]:THR:CG2	1:A:50:HIS:H	2.28	0.42
1:C:40:ARG:HH12	1:C:42:GLU:CD	2.23	0.42
1:C:234:ARG:NE	2:C:310:HOH:O	2.51	0.42
1:A:248:ARG:NH2	2:A:383:HOH:O	2.36	0.42
1:B:47[B]:THR:HG21	1:B:160:LYS:O	2.20	0.42
1:B:47[A]:THR:CG2	1:B:50:HIS:H	2.31	0.42
1:C:6:ILE:CD1	1:C:88:LEU:HD23	2.50	0.42
1:C:88:LEU:HD11	1:C:116:ILE:HD12	2.01	0.41
1:B:100:ARG:NH2	2:B:302:HOH:O	2.53	0.41
1:C:47[A]:THR:HG21	1:C:50:HIS:HB2	1.98	0.41
1:A:103:TYR:HD1	2:A:311:HOH:O	2.03	0.41
1:C:47[B]:THR:HG21	1:C:160:LYS:O	2.20	0.41
1:C:121:MSE:HB3	1:C:124:ILE:HD13	2.02	0.41
1:B:27:ARG:HD2	2:B:322:HOH:O	2.21	0.41
1:C:47[A]:THR:HG1	1:C:48:THR:H	1.68	0.41
1:C:32:ASN:HB3	2:C:287:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD21	1:A:175:VAL:CG2	2.51	0.41
1:B:250:GLN:NE2	1:C:161:LEU:HB2	2.36	0.41
1:A:106:LEU:HD22	1:A:252:ILE:HD11	2.03	0.41
1:A:98:LEU:HD22	1:A:132:ILE:HD12	2.03	0.41
1:A:239:ASP:HA	1:A:240:PRO:HD2	1.94	0.41
1:C:106:LEU:HD22	1:C:252:ILE:HD11	2.02	0.40
1:C:106:LEU:HD21	1:C:175:VAL:CG2	2.51	0.40
1:C:51:GLN:HG2	2:C:307:HOH:O	2.20	0.40
1:A:216:ARG:CZ	2:A:326:HOH:O	2.69	0.40
1:B:11:ASN:HA	1:B:60:THR:O	2.22	0.40
1:A:124:ILE:HG21	2:A:297:HOH:O	2.22	0.40
1:A:9:ILE:HG12	1:A:104:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:358:HOH:O	2:A:358:HOH:O[2_555]	1.89	0.31

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/270 (94%)	247 (97%)	7 (3%)	0	100	100
1	B	253/270 (94%)	246 (97%)	7 (3%)	0	100	100
1	C	253/270 (94%)	246 (97%)	7 (3%)	0	100	100
All	All	760/810 (94%)	739 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/224 (95%)	200 (94%)	13 (6%)	23	26
1	B	212/224 (95%)	201 (95%)	11 (5%)	29	33
1	C	212/224 (95%)	201 (95%)	11 (5%)	29	33
All	All	637/672 (95%)	602 (94%)	35 (6%)	26	30

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	8	LEU
1	A	32	ASN
1	A	36	VAL
1	A	74	GLU
1	A	82	LEU
1	A	121	MSE
1	A	134	ILE
1	A	166	TYR
1	A	224	GLN
1	A	238	ASP
1	A	239	ASP
1	A	242	LEU
1	B	5	THR
1	B	8	LEU
1	B	32	ASN
1	B	36	VAL
1	B	74	GLU
1	B	82	LEU
1	B	122	LEU
1	B	166	TYR
1	B	238	ASP
1	B	239	ASP
1	B	242	LEU
1	C	5	THR
1	C	8	LEU

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Mol	Chain	Res	Type
1	C	32	ASN
1	C	36	VAL
1	C	121	MSE
1	C	122	LEU
1	C	134	ILE
1	C	190	LYS
1	C	238	ASP
1	C	239	ASP
1	C	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	32	ASN
1	A	50	HIS
1	A	79	HIS
1	A	91	ASN
1	A	128	GLN
1	A	129	ASN
1	A	200	GLN
1	B	32	ASN
1	B	79	HIS
1	B	91	ASN
1	B	128	GLN
1	B	179	GLN
1	B	200	GLN
1	B	243	HIS
1	C	11	ASN
1	C	32	ASN
1	C	79	HIS
1	C	91	ASN
1	C	128	GLN
1	C	200	GLN
1	C	243	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/270 (92%)	0.41	12 (4%) 34 34	3, 17, 44, 62	1 (0%)
1	B	249/270 (92%)	0.35	11 (4%) 38 37	3, 17, 44, 62	0
1	C	249/270 (92%)	0.43	22 (8%) 12 11	3, 17, 44, 62	0
All	All	747/810 (92%)	0.40	45 (6%) 25 25	3, 17, 44, 62	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ILE	7.6
1	B	239	ASP	4.7
1	C	239	ASP	4.6
1	A	195	ASP	4.4
1	C	213	ILE	4.4
1	C	195	ASP	4.1
1	A	233	LEU	4.0
1	C	231	ALA	3.9
1	C	71	SER	3.7
1	C	216	ARG	3.7
1	C	233	LEU	3.6
1	A	239	ASP	3.6
1	B	238	ASP	3.5
1	A	193	PRO	3.5
1	C	196	ILE	3.5
1	C	230	LEU	3.2
1	A	213	ILE	3.2
1	A	191	VAL	3.1
1	B	186	ASP	3.0
1	B	194	SER	2.9
1	A	218[A]	TYR	2.8
1	C	222	ALA	2.8
1	C	34	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	129	ASN	2.5
1	C	193	PRO	2.5
1	A	127	LYS	2.4
1	C	186	ASP	2.4
1	B	127	LYS	2.4
1	C	128	GLN	2.3
1	A	211	GLY	2.3
1	C	234	ARG	2.2
1	C	191	VAL	2.2
1	C	236	GLU	2.2
1	C	227	ASP	2.2
1	B	229	ALA	2.2
1	B	213	ILE	2.2
1	C	190	LYS	2.2
1	C	235	ASN	2.2
1	C	127	LYS	2.1
1	B	103	TYR	2.1
1	B	74	GLU	2.1
1	C	224	GLN	2.1
1	A	74	GLU	2.0
1	B	71	SER	2.0
1	A	216	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.